

CELANESE CHEMICAL COMPANY, INC.
TECHNICAL CENTER
Corpus Christi, Texas

DDD-38-81
WNU-17-81

Redox II Design and Economics Update

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Redox Technologies, Inc.
Design
Economics
Update
Ethylene Glycol
Process
Comparison
Redox II
Syn Gas
Shell
Purification
Acetone
Glycerine
Propylene Glycol

* Summary only
** With appendices

S/N 642

CELANESE CHEMICAL COMPANY, INC.
TECHNICAL CENTER
Corpus Christi, Texas

To: W. E. Heinz

From: D. D. Dickinson
W. N. Uber

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Redox II Design and Economics Update

SUMMARY

A detailed design and economic update for the Redox II ethylene glycol (EG) process shows a moderate (5%) NSR advantage over Shell. A more attractive R&D target case (higher EG wt%) has a 14% advantage over Shell. These results are summarized below for 500 MM lb/yr EG units (1989 construction, 1990 operation):

	REDOX II			
	Base Case	R & D Target	Shell	CZ Syn Gas
Raw material cost, contained EG (a)	39.1	39.1	62.8	22.4
TFC, \$MM	319	278	265	525
TFC contribution, c/lb EG	19.8	17.3	16.1	48.0
Raw materials, c/lb	69.8	73.0	64.3	31.4
By-products, c/lb				
Glycerine	(4.3)	(4.3)		(20.9)
Acetone	(14.8)	(19.3)		
t-Butanol	(6.3)	(2.1)		
Ethanol	(3.0)	(10.1)		
Others	(4.8)	(3.3)	(9.0)	(8.3)
-----	-----	-----	-----	-----
Totals	(33.2)	(39.1)	(9.0)	(29.2)
Utilities, c/lb	21.2	17.2	8.5	13.8
Cat & Chem, c/lb	0.1	0.1	1.8	3.8
ENSR , c/lb EG	79.5	71.3	83.3	71.1
Shutdown NSR			63.8 (b)	

(a) No byproducts, Shell @ 70% effy, others @ 100% effy

(b) Shell shutdown NSR as zero cash flow

APPENDIX B
BLOCK 2 - TBHP ALKYLATION

- Table B-I: Capital/Utilities Summary
- Figure B-1: Process Flow Diagram
- Table B-II: Block Capital Estimate
- Table B-III: Block Material Balance

Process Description

T-butyl-hydroperoxide (TBHP) is alkylated with isobutylene to DTBP in the liquid phase in the presence of strong acid ion exchange resin. Low temperature (70°C) helps ensure resin stability, while maintaining rates (30 min. res. time). Excess isobutylene (23%) ensures complete TBHP conversion in the plug flow reactor.

Excess isobutylene is removed in a single distillation step. Low base temperature of 115°C prevents DTBP decomposition. Product DTBP is immediately cooled and stored for feed to the Redox reactor.

TABLE B-I
CAPITAL/UTILITIES SUMMARY

Block 2--TBHP Alkylation

TFC (1977 MSI): \$ 9.6 MM

	Units/lb EG -----
Electricity, KWH	0.0015
Steam, lb: S-15	0.06
Cooling Water, gal	0.8

FIGURE B-1
BLOCK 2 -- TBHP ALKYLATION
Detailed Process Flow Diagram

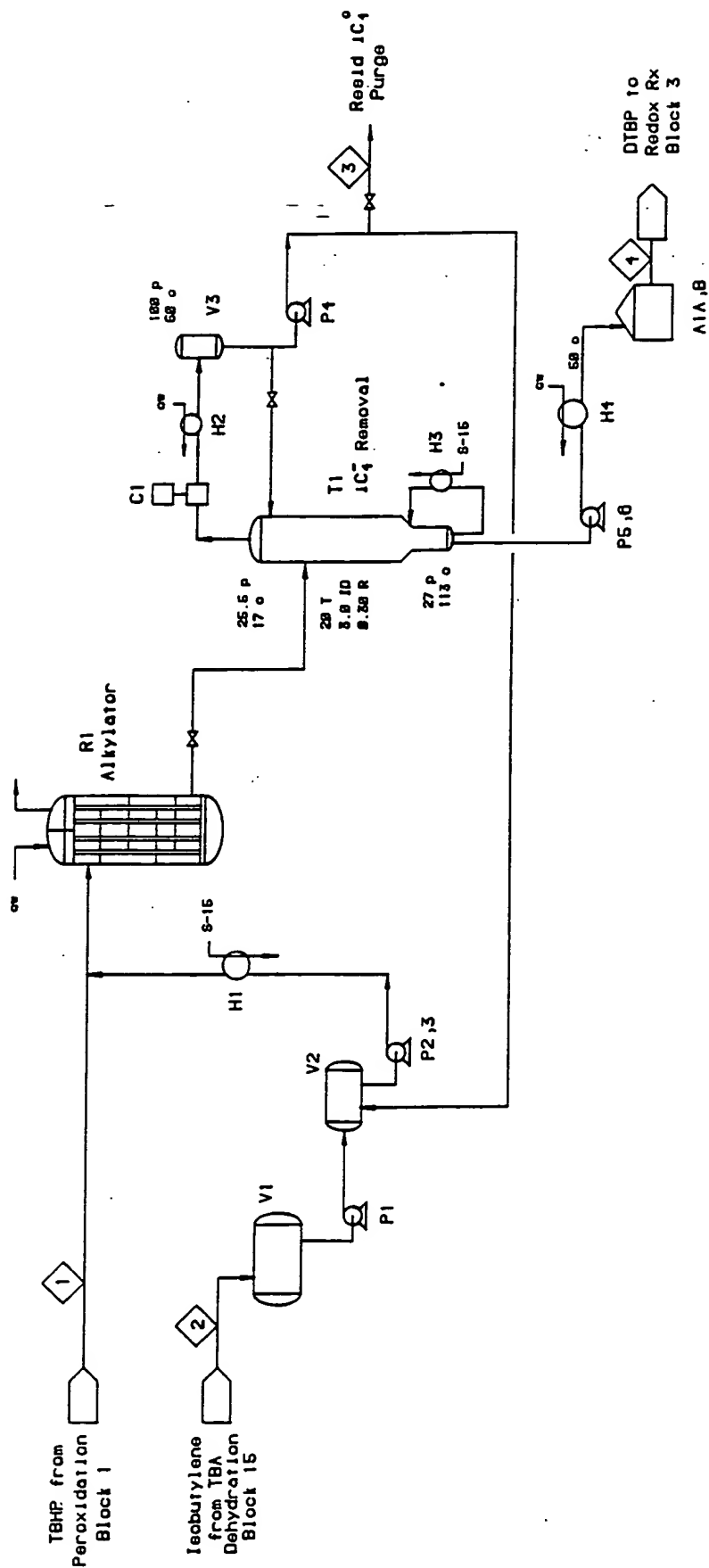


TABLE B-II

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REDOX II // ALKYLATION--BLOCK 2
 ODD/MAY 13 1981

 *
 * SUMMARY OF RESULTS *
 *

CASE STUDY FOR PLANT CAPACITY TIMES 1.49

YEAR= 1981
 MSI= 1877
 BASE MSI= 670

EQUIPMENT TYPE	DELIVERED EQUIPMENT COST M\$	RL/DEC RATIO	BATTERY LIMITS COST M\$
VESSELS	288.68	5.09	1469.15
ATM TANKS	333.72	2.55	850.56
TOWERS	83.36	5.89	490.79
XCHANGERS	1485.47	1.91	2830.08
PUMPS	47.16	10.75	507.10
COMPRESSORS	102.77	3.46	356.07
BLOWERS/FANS	0.00	0.00	0.00
FURNACES/BOILERS	0.00	0.00	0.00
REFRIGERATION	0.00	0.00	0.00
MISCELLANEOUS	0.00	0.00	0.00

*** TOTALS 2341.16 2.78 6503.75

BATTERY LIMITS PLUS 20.0 PERCENT CONTINGENCY IS:
 (CONTINGENCY IS OVERALL PROCESS AND ESTIMATING)

7804.49

 *
 * TOTAL PLANT (BATTERY LIMITS) *
 *

CASE STUDY FOR PLANT CAPACITY TIMES 1.49

	DELIVERED EQUIPMENT (MS)	DIRECT LABOR (MS)	INSULATION AND PAINT (MS)	PIPING (MS)	INSTRMNTS (MS)	ELECTRCL (MS)	CIVIL (MS)	ENG/CONS OVHD (MS)	TOTAL (BL) (MS)	BL/DEC RATIO
VESSELS	288.68	6.78	125.54	110.10	179.20	48.66	179.22	530.95	1469.15	5.09
ATM TANKS	333.72	6.74	22.69	57.43	27.87	49.74	104.09	248.28	850.56	2.55
TOWERS	83.36	1.77	11.85	157.46	61.41	3.02	26.45	145.47	490.79	5.89
HEAT EXCHANGERS	1485.47	27.87	36.69	158.72	93.53	61.88	337.30	628.62	2830.08	1.91
PUMPS	47.16	2.18	5.09	90.23	7.00	58.21	54.06	243.17	507.10	10.75
COMPRESSORS	102.77	2.52	5.61	16.19	26.92	44.09	37.01	120.96	356.07	3.46
BLOWERS/FANS	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FURNACES/BOILERS	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
REFRIGERATION	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MISCELLANEOUS	0.00	0.00	0.00	6.97	0.00	0.00	0.00	0.00	6.97	0.00
*** TOTAL	2341.16	47.86	207.47	597.11	395.94	265.59	738.14	1917.44	6510.71	
PERCENT DEC	100.00	2.04	8.86	25.50	16.91	11.34	31.53	81.90	278.10	
PERCENT HL	35.96	.74	3.19	9.17	6.08	4.08	11.34	29.45	100.00	

TABLE B-III

BLOCK 2: TBHP ALKYLATION TO DTBP

BLOCK STREAM 1: TBHP/TBA FROM PEPOXIDATION
-- FEED STREAM FROM BLOCK 1 --

*** S- 5 ***

METHANE =	0.000000	METHANOL=	8.540131	METHYLAL=	0.000000
CRB DIOX=	0.000000	TBUTANOL=	137.897213	GLYCOALD=	0.000000
HYDROGN =	0.000000	ETH GLY =	0.000000	ETHANOL =	0.000000
OXYGEN =	0.000000	GLYCERIN=	0.000000	CRB MNOX=	0.000000
I-BUTANE=	0.248960	TBHP =	280.159745	12PRDIOL=	0.000000
N-BUTANE=	0.414374	DTBP =	0.000000	13PRDIOL=	0.000000
I-BUTENE=	0.000000	TETRAOL =	0.000000	ME ETHER=	0.000000
MEFORMAT=	0.000000	WATER =	21.550750	CYHEXANE=	0.000000
ACETONE =	8.550475	FORMALD =	0.000000	NA HCO3 =	0.000000

TOTAL MOL = 457.361648
TOTAL WGT = 36665.9863
AVERG MWT = 80.1684760

BLOCK STREAM 2: ISOBUTYLENE FEED
-- RECYCLE STREAM FROM BLOCK 15 --

*** S- 9 ***

METHANE =	1.407838	METHANOL=	0.000000	METHYLAL=	0.000000
CRB DIOX=	0.000000	TBUTANOL=	0.042024	GLYCOALD=	0.000000
HYDROGN =	0.000000	ETH GLY =	0.000000	ETHANOL =	0.000000
OXYGEN =	0.000000	GLYCERIN=	0.000000	CRB MNOX=	0.000000
I-BUTANE=	0.000000	TBHP =	0.000000	12PRDIOL=	0.000000
N-BUTANE=	0.000000	DTBP =	0.000000	13PRDIOL=	0.000000
I-BUTENE=	280.159745	TETRAOL =	0.000000	ME ETHER=	0.000000
MEFORMAT=	0.000000	WATER =	1.400799	CYHEXANE=	0.000000
ACETONE =	1.407838	FORMALD =	0.000000	NA HCO3 =	0.000000

TOTAL MOL = 284.418244
TOTAL WGT = 15850.7829
AVERG MWT = 55.7305421

BLOCK STREAM 3: RESIDUAL ISOBUTANE PURGE
-- EXTERNAL FUEL STREAM --

*** S- 10 ***

METHANE =	1.407838	METHANOL=	0.004782	METHYLAL=	0.000000
CRB DIOX=	0.000000	TBUTANOL=	0.004138	GLYCOALD=	0.000000
HYDROGN =	0.000000	ETH GLY =	0.000000	ETHANOL =	0.000000
OXYGEN =	0.000000	GLYCERIN=	0.000000	CRB MNOX=	0.000000
I-BUTANE=	0.208180	TBHP =	0.000000	12PRDIOL=	0.000000
N-BUTANE=	0.222167	DTBP =	0.000000	13PRDIOL=	0.000000
I-BUTENE=	0.000000	TETRAOL =	0.000000	ME ETHER=	0.000000
MEFORMAT=	0.000000	WATER =	0.000000	CYHEXANE=	0.000000
ACETONE =	0.014937	FORMALD =	0.000000	NA HCO3 =	0.000000

TOTAL MOL = 1.86206386
TOTAL WGT = 48.9250136
AVERG MWT = 26.2746165

BLOCK STREAM 4 : DTBP/TBA PRODUCT TO REDOX RX
 -- PRODUCT STREAM TO BLOCK 3 --

```

*** S- 11 ***
METHANE = 0.000000 METHANOL= 8.535349 METHYLAL= 0.000000
CRB DIOX= 0.000000 TBUTANOL= 137.935098 GLYCOALD= 0.000000
HYDROGN = 0.000000 ETH GLY = 0.000000 ETHANOL = 0.000000
OXYGEN = 0.000000 GLYCERIN= 0.000000 CRB MNOX= 0.000000
I-BUTANE= 0.040760 TBHP = 0.000000 12PRDIOL= 0.000000
N-BUTANE= 0.192187 DTBP = 280.159745 13PRDIOL= 0.000000
I-BUTENE= 0.000000 TETRAOL = 0.000000 ME ETHER= 0.000000
MEFORMAT= 0.000000 WATER = 22.951548 CYHEXANE= 0.000000
ACETONE = 9.943376 FORMALD = 0.000000 NA HCO3 = 0.000000
-----
TOTAL MOL = 459.758083
TOTAL WGT = 52467.8442
AVERG MWT = 114.120548
  
```

BLOCK STREAM 5 : RX STOICHIOMETRY
 -- INTERNAL REFERENCE STREAM --

```

*** S- 12 ***
METHANE = 0.000000 METHANOL= 0.000000 METHYLAL= 0.000000
CRB DIOX= 0.000000 TBUTANOL= 0.000000 GLYCOALD= 0.000000
HYDROGN = 0.000000 ETH GLY = 0.000000 ETHANOL = 0.000000
OXYGEN = 0.000000 GLYCERIN= 0.000000 CRB MNOX= 0.000000
I-BUTANE= 0.000000 TBHP = -1.000000 12PRDIOL= 0.000000
N-BUTANE= 0.000000 DTBP = 1.000000 13PRDIOL= 0.000000
I-BUTENE= -1.000000 TETRAOL = 0.000000 ME ETHER= 0.000000
MEFORMAT= 0.000000 WATER = 0.000000 CYHEXANE= 0.000000
ACETONE = 0.000000 FORMALD = 0.000000 NA HCO3 = 0.000000
-----
TOTAL MOL = -1.00000000
TOTAL WGT = 0.000000000E+00
AVERG MWT = 0.000000000E+00
  
```

BLOCK STREAM 6 : RX FEED
 -- INTERNAL REFERENCE STREAM --

```

*** S- 13 ***
METHANE = 1.407638 METHANOL= 8.540131 METHYLAL= 0.000000
CRB DIOX= 0.000000 TBUTANOL= 137.939237 GLYCOALD= 0.000000
HYDROGN = 0.000000 ETH GLY = 0.000000 ETHANOL = 0.000000
OXYGEN = 0.000000 GLYCERIN= 0.000000 CRB MNOX= 0.000000
I-BUTANE= 0.248960 TBHP = 280.159745 12PRDIOL= 0.000000
N-BUTANE= 0.414374 DTBP = 0.000000 13PRDIOL= 0.000000
I-BUTENE= 280.159745 TETRAOL = 0.000000 ME ETHER= 0.000000
MEFORMAT= 0.000000 WATER = 22.951548 CYHEXANE= 0.000000
ACETONE = 9.958313 FORMALD = 0.000000 NA HCO3 = 0.000000
-----
TOTAL MOL = 741.779891
TOTAL WGT = 52516.7692
AVERG MWT = 70.7963167
  
```

BLOCK 2 MASS BAL, PRGD-FEED WGT : 0.000000000E+00